Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH +)	-0.33	±0.82 (n=50)
logP (neutral X)	2.12	±0.01 (n=50)
RMSD	0.537	

18C-09010 Points 1 to 24

M11_octanol concentration factor	0.962
Carbonate	0.0600 mM
Acidity error	-0.46392 mM

18C-09010 Points 25 to 45

M11_octanol concentration factor	0.930
Carbonate	0.0890 mM
Acidity error	-0.75734 mM

18C-09010 Points 46 to 69

M11_octanol concentration factor	0.907
Carbonate	0.1290 mM
Acidity error	-0.81079 mM

Warnings and errors

Errors	None
Warnings	None

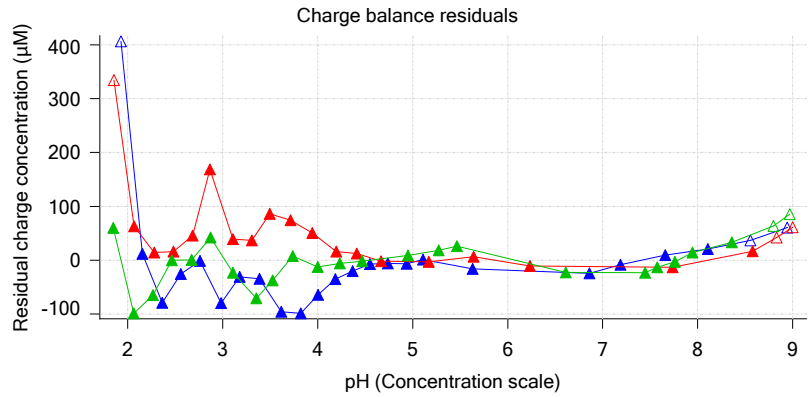
Sample logD and percent species

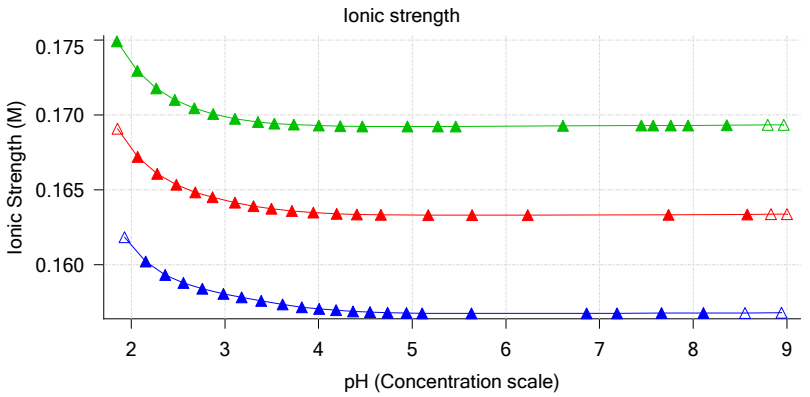
pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	-0.20	61.06 %	0.08 %	28.50 %	10.36 %	
1.200	-0.13	57.55 %	0.12 %	26.86 %	15.48 %	Stomach pH
2.000	0.33	31.48 %	0.41 %	14.69 %	53.42 %	
3.000	1.19	5.39 %	0.69 %	2.51 %	91.40 %	
4.000	1.87	0.58 %	0.75 %	0.27 %	98.40 %	
5.000	2.09	0.06 %	0.75 %	0.03 %	99.16 %	
6.000	2.12	0.01 %	0.75 %	0.00 %	99.24 %	
6.500	2.12	0.00 %	0.75 %	0.00 %	99.24 %	
7.000	2.12	0.00 %	0.75 %	0.00 %	99.25 %	
7.400	2.12	0.00 %	0.75 %	0.00 %	99.25 %	Blood pH
8.000	2.12	0.00 %	0.75 %	0.00 %	99.25 %	
9.000	2.12	0.00 %	0.75 %	0.00 %	99.25 %	
10.000	2.12	0.00 %	0.75 %	0.00 %	99.25 %	
11.000	2.12	0.00 %	0.75 %	0.00 %	99.25 %	
12.000	2.12	0.00 %	0.75 %	0.00 %	99.25 %	

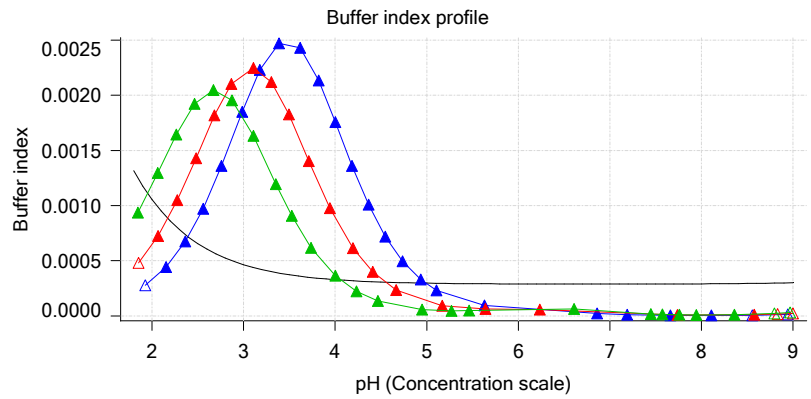
Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

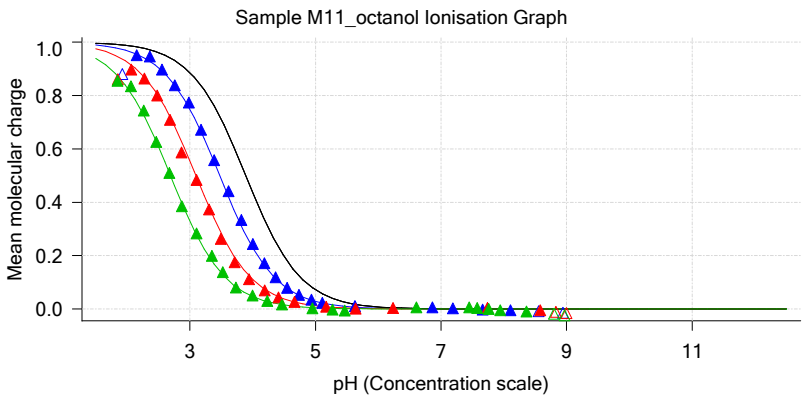
Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

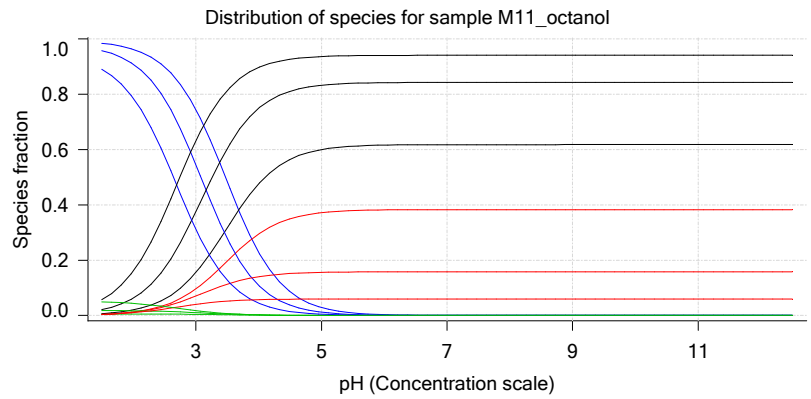
Graphs

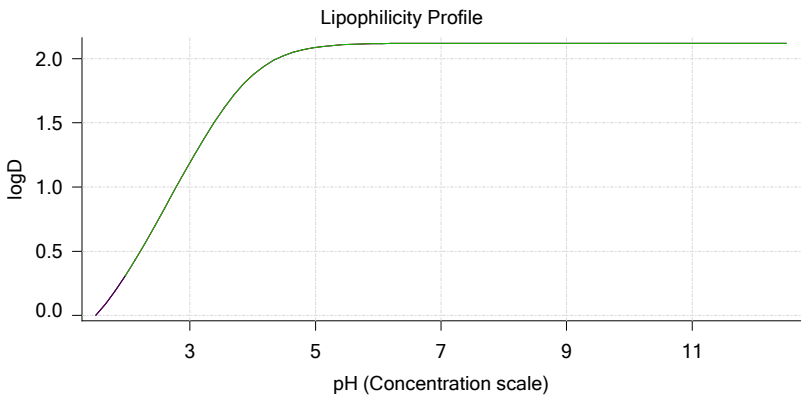


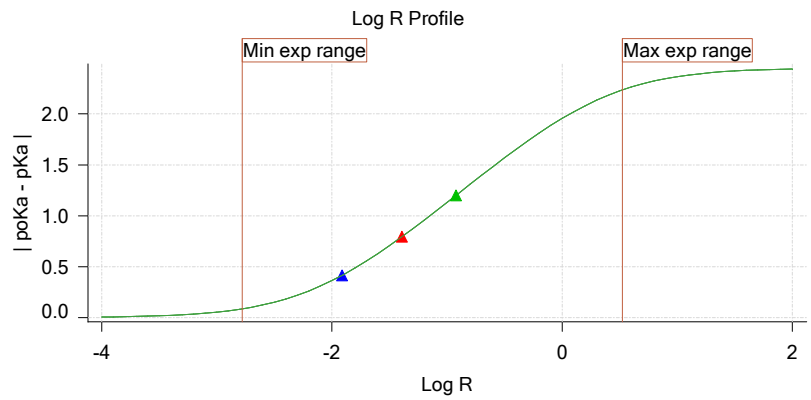


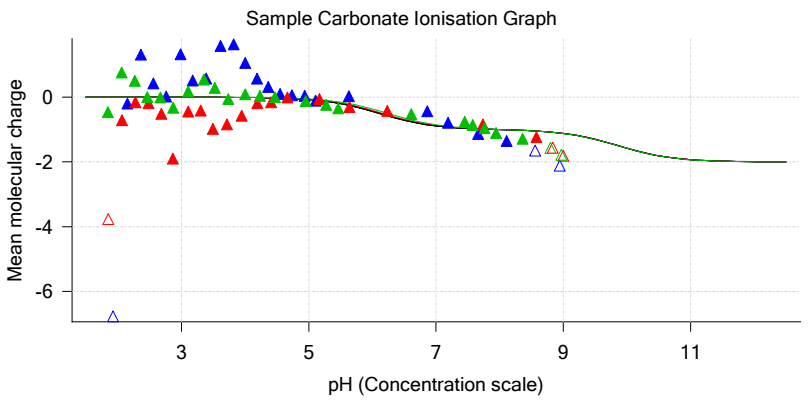








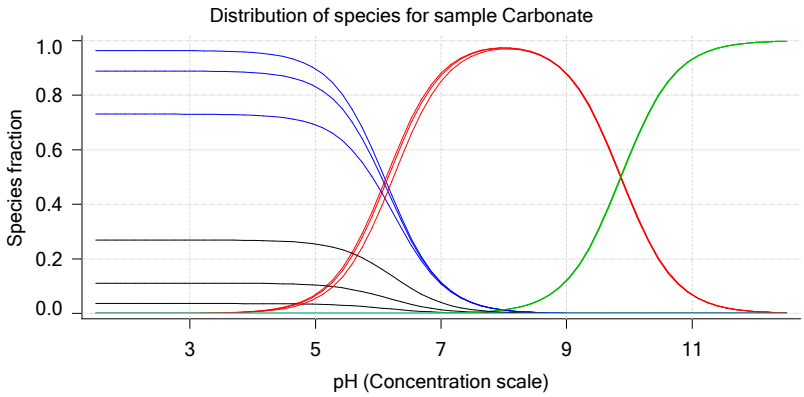




Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)



Sample name:	**M11_octanol**	Experiment start time:	**3/9/2018 4:01:24 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-09010**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 1 of 3 18C-09010 Points 1 to 24

Overall results

RMSD	0.632
Average ionic strength	0.157 M
Average temperature	24.9°C
Partition ratio	0.0123 : 1
Analyte concentration range	4427.7 µM to 4566.6 µM
Total points considered	21 of 24

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.102	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
S	0.9967	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
jH	1.2	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
jOH	0.0	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r

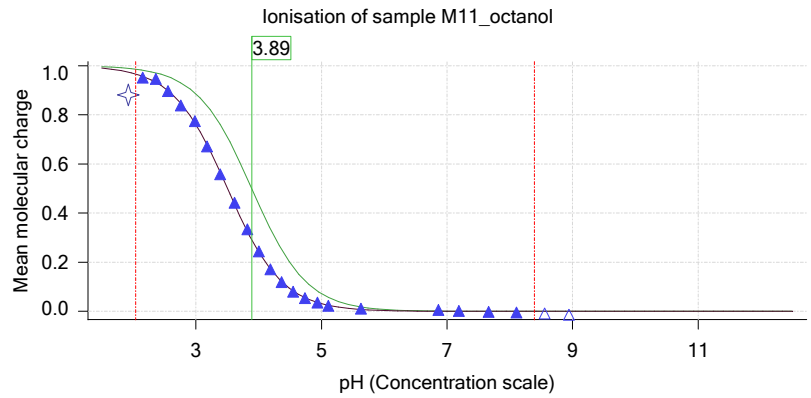
Titrants

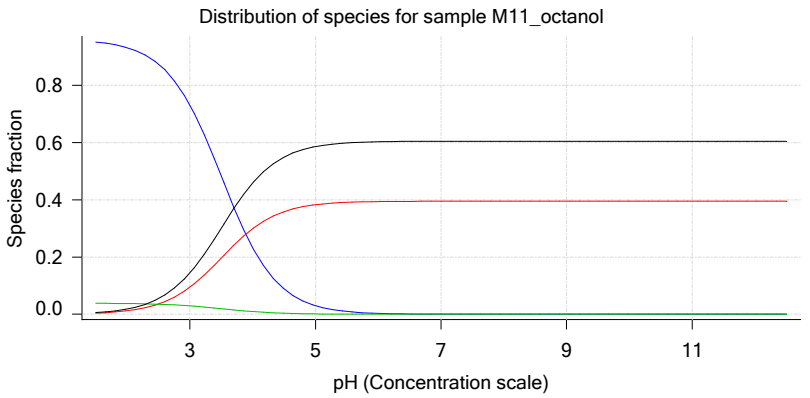
0.50 M HCl	0.999843	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
0.50 M KOH	0.999845	3/9/2018 4:01:24 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M11_octanol concentration factor	0.962
Base pKa 1	3.89
logP (XH +)	0.52
logP (neutral X)	2.10

Sample graphs

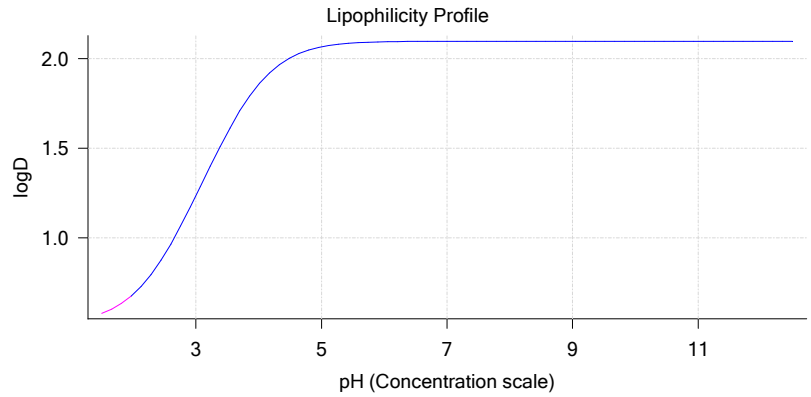




Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



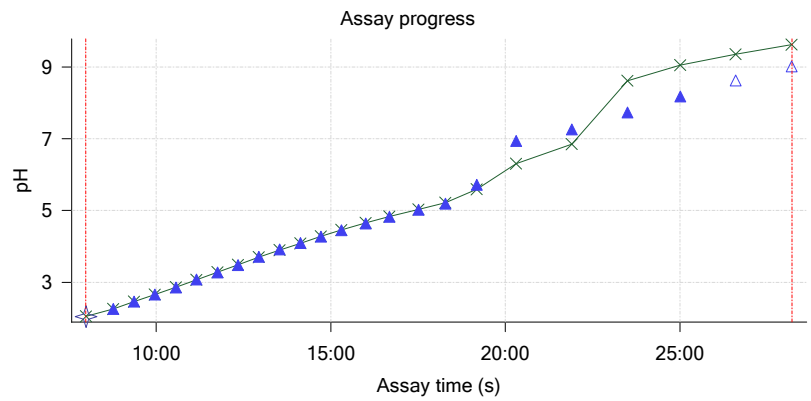
Sample logD and percent species

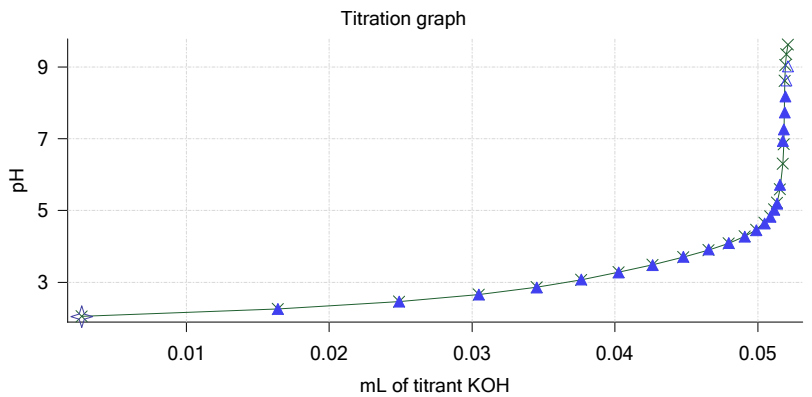
pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	0.54	95.82 %	0.12 %	3.86 %	0.19 %	
1.200	0.55	95.65 %	0.20 %	3.86 %	0.30 %	Stomach pH
2.000	0.68	93.20 %	1.20 %	3.76 %	1.84 %	
3.000	1.23	73.19 %	9.43 %	2.95 %	14.43 %	
4.000	1.86	23.25 %	29.95 %	0.94 %	45.86 %	
5.000	2.07	2.97 %	38.29 %	0.12 %	58.62 %	
6.000	2.09	0.31 %	39.39 %	0.01 %	60.30 %	
6.500	2.10	0.10 %	39.47 %	0.00 %	60.43 %	
7.000	2.10	0.03 %	39.50 %	0.00 %	60.47 %	
7.400	2.10	0.01 %	39.51 %	0.00 %	60.48 %	Blood pH
8.000	2.10	0.00 %	39.51 %	0.00 %	60.49 %	
9.000	2.10	0.00 %	39.51 %	0.00 %	60.49 %	
10.000	2.10	0.00 %	39.51 %	0.00 %	60.49 %	
11.000	2.10	0.00 %	39.51 %	0.00 %	60.49 %	
12.000	2.10	0.00 %	39.51 %	0.00 %	60.49 %	

Carbonate and acidity

Carbonate 0.060 mM
Acidity error -0.464 mM

Other graphs

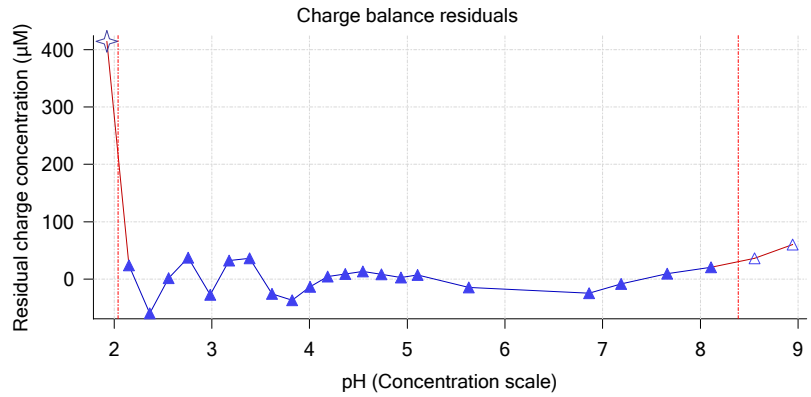


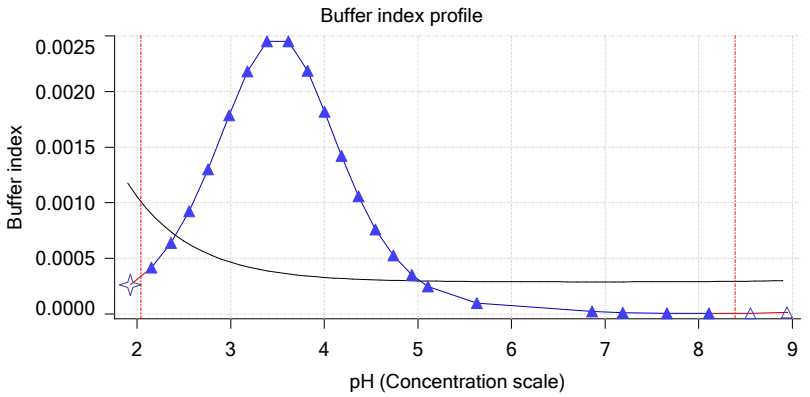


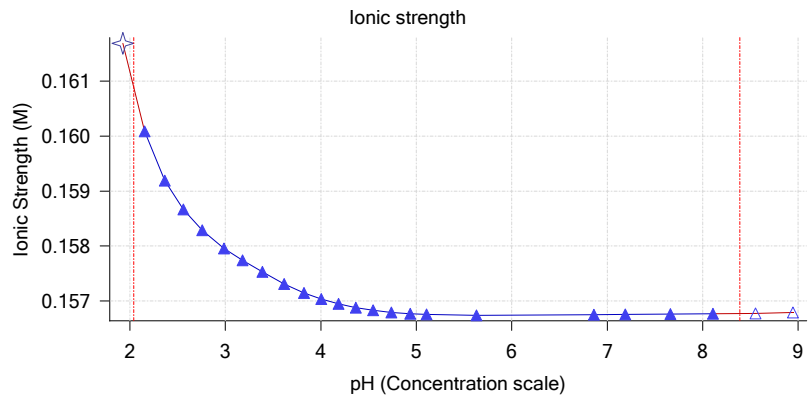
Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

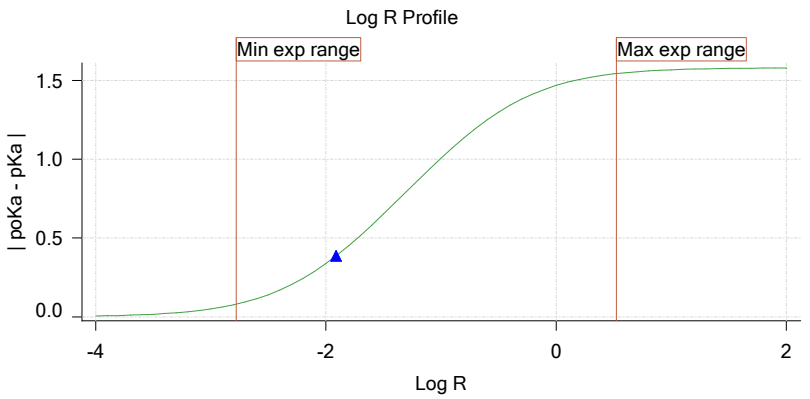
Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

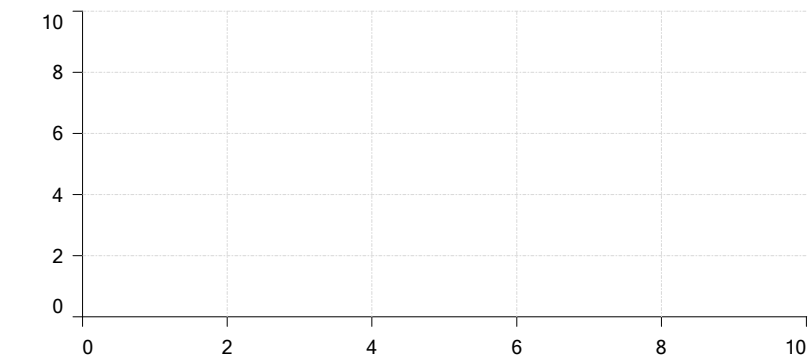
Other graphs (continued)

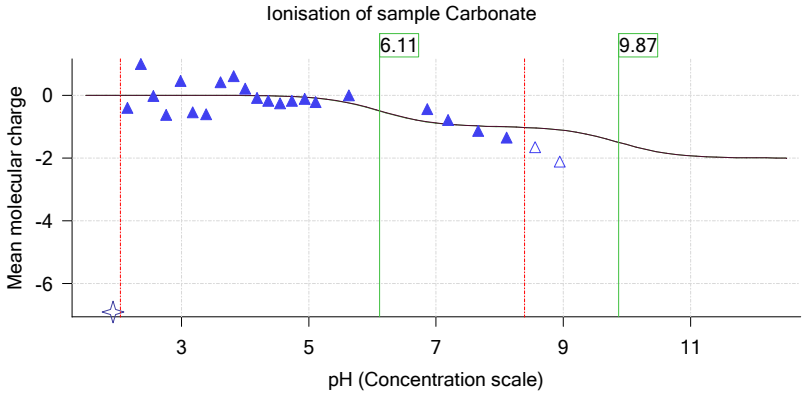












Sample name:	**M11_octanol**	Experiment start time:	**3/9/2018 4:01:24 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-09010**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 2 of 3 18C-09010 Points 25 to 45

Overall results

RMSD	0.373
Average ionic strength	0.164 M
Average temperature	25.0°C
Partition ratio	0.0405 : 1
Analyte concentration range	4011.7 µM to 4147.6 µM
Total points considered	18 of 21

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.102	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
S	0.9967	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
jH	1.2	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
jOH	0.0	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r

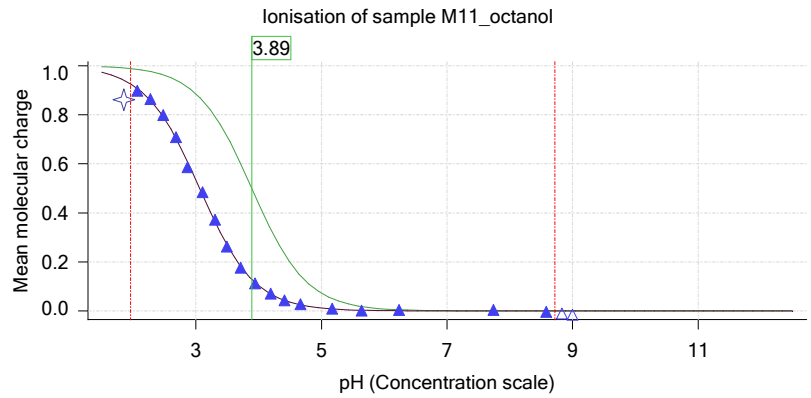
Titrants

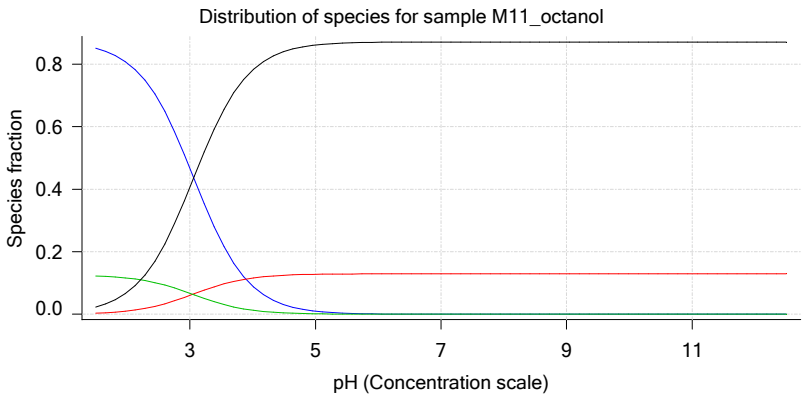
0.50 M HCl	0.999843	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
0.50 M KOH	0.999845	3/9/2018 4:01:24 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M11_octanol concentration factor	0.930
Base pKa 1	3.89
logP (XH +)	0.55
logP (neutral X)	2.22

Sample graphs

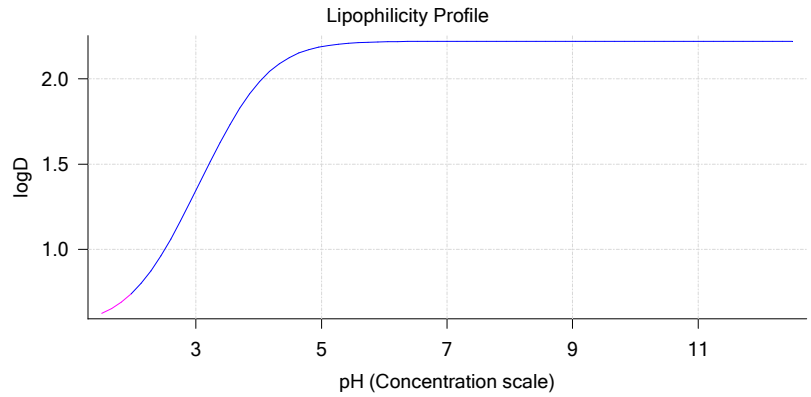




Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



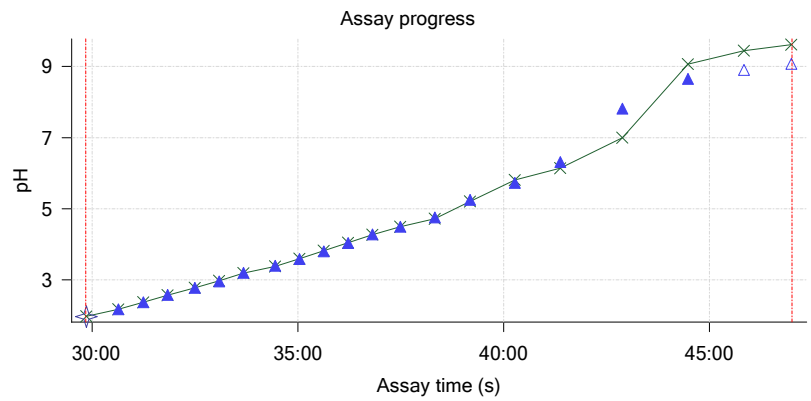
Sample logD and percent species

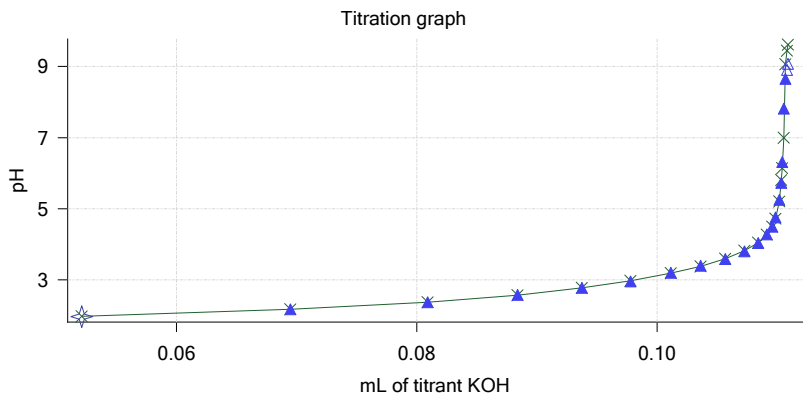
pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	0.57	86.67 %	0.11 %	12.47 %	0.75 %	
1.200	0.59	86.23 %	0.18 %	12.40 %	1.19 %	Stomach pH
2.000	0.75	80.41 %	1.04 %	11.57 %	6.98 %	
3.000	1.34	46.71 %	6.02 %	6.72 %	40.55 %	
4.000	1.98	9.00 %	11.59 %	1.29 %	78.12 %	
5.000	2.19	0.99 %	12.77 %	0.14 %	86.09 %	
6.000	2.22	0.10 %	12.91 %	0.01 %	86.98 %	
6.500	2.22	0.03 %	12.92 %	0.00 %	87.05 %	
7.000	2.22	0.01 %	12.92 %	0.00 %	87.07 %	
7.400	2.22	0.00 %	12.92 %	0.00 %	87.08 %	Blood pH
8.000	2.22	0.00 %	12.92 %	0.00 %	87.08 %	
9.000	2.22	0.00 %	12.92 %	0.00 %	87.08 %	
10.000	2.22	0.00 %	12.92 %	0.00 %	87.08 %	
11.000	2.22	0.00 %	12.92 %	0.00 %	87.08 %	
12.000	2.22	0.00 %	12.92 %	0.00 %	87.08 %	

Carbonate and acidity

Carbonate 0.089 mM
Acidity error -0.757 mM

Other graphs

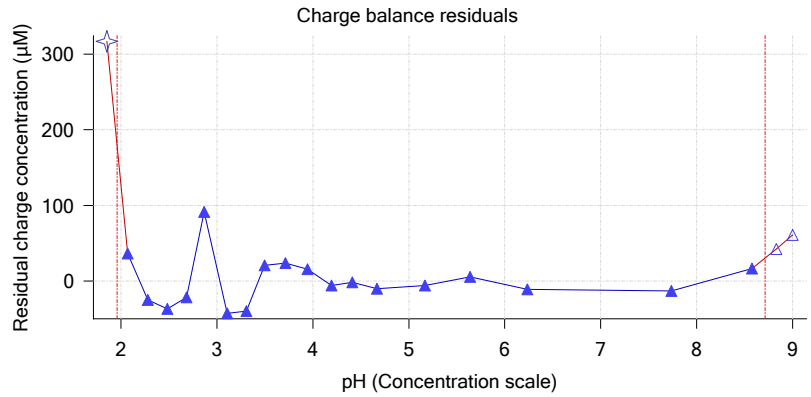


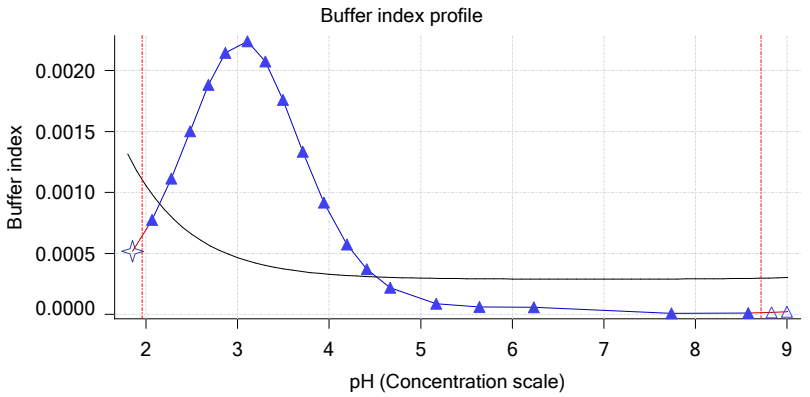


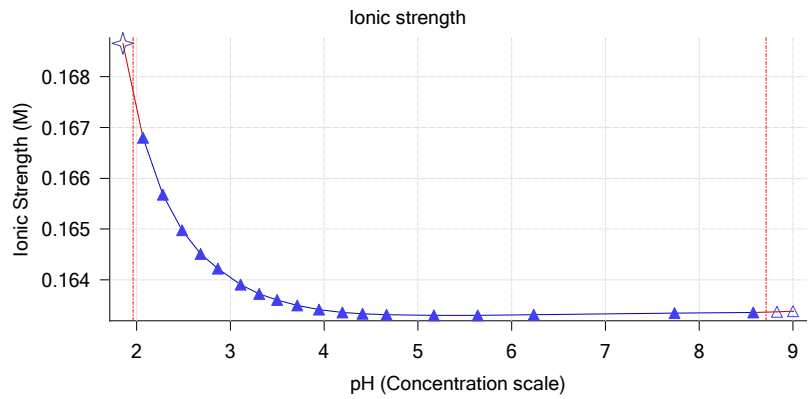
Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

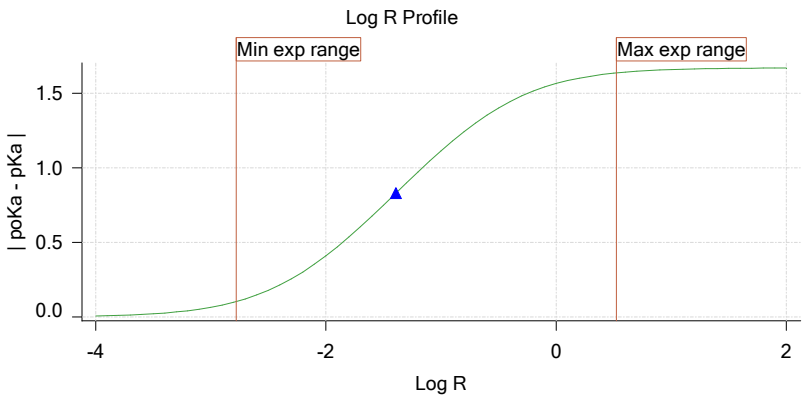
Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

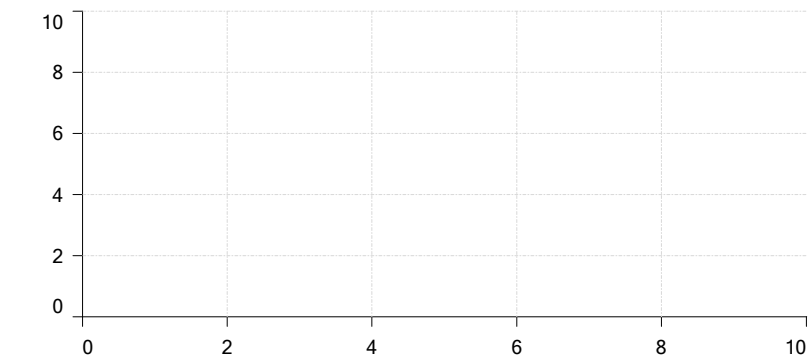
Other graphs (continued)

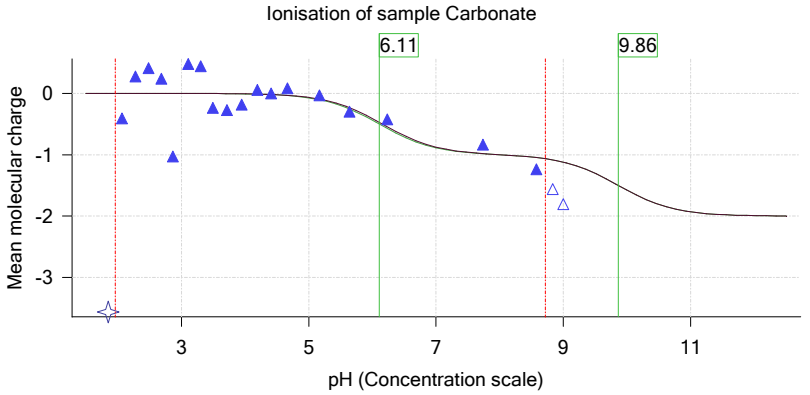












Sample name:	**M11_octanol**	Experiment start time:	**3/9/2018 4:01:24 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-09010**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 3 of 3 18C-09010 Points 46 to 69

Overall results

RMSD	0.548
Average ionic strength	0.170 M
Average temperature	25.0°C
Partition ratio	0.1193 : 1
Analyte concentration range	3477.2 µM to 3586.0 µM
Total points considered	22 of 24

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.102	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
S	0.9967	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
jH	1.2	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
jOH	0.0	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r

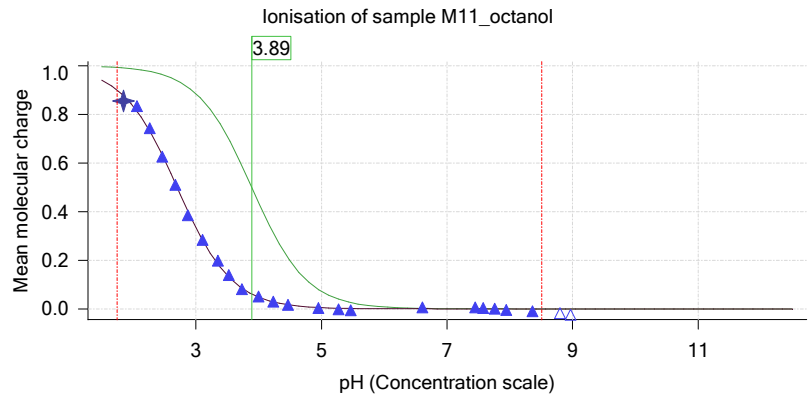
Titrants

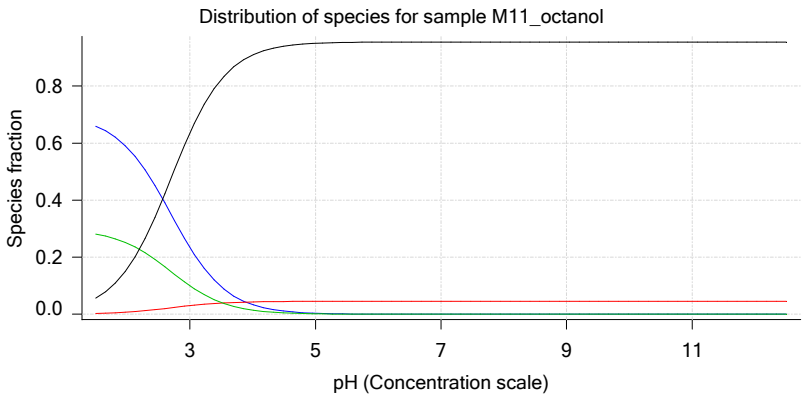
0.50 M HCl	0.999843	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
0.50 M KOH	0.999845	3/9/2018 4:01:24 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M11_octanol concentration factor	0.907
Base pKa 1	3.89
logP (XH +)	0.55
logP (neutral X)	2.25

Sample graphs

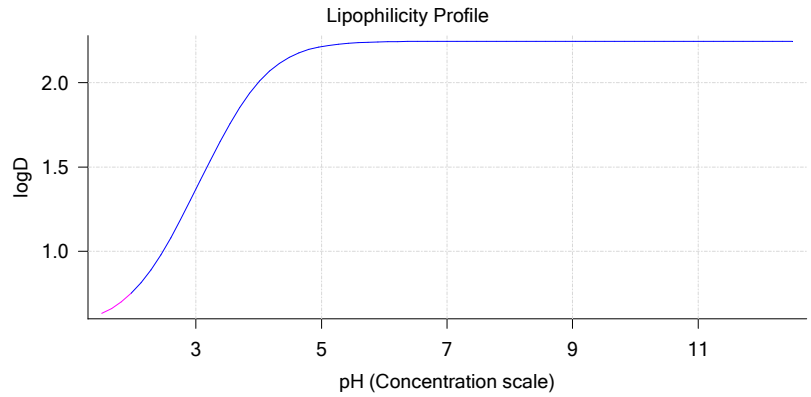




Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



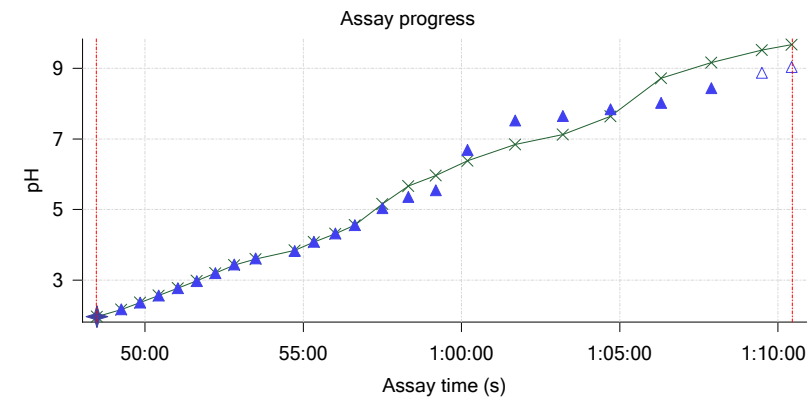
Sample logD and percent species

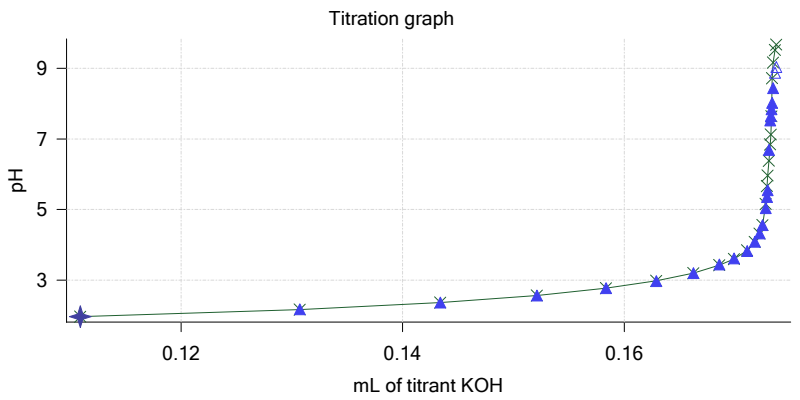
pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	0.58	68.74 %	0.09 %	29.31 %	1.86 %	
1.200	0.59	67.97 %	0.14 %	28.98 %	2.92 %	Stomach pH
2.000	0.76	58.48 %	0.75 %	24.93 %	15.84 %	
3.000	1.37	23.45 %	3.02 %	10.00 %	63.53 %	
4.000	2.00	3.36 %	4.32 %	1.43 %	90.89 %	
5.000	2.21	0.35 %	4.52 %	0.15 %	94.98 %	
6.000	2.24	0.04 %	4.54 %	0.02 %	95.41 %	
6.500	2.25	0.01 %	4.54 %	0.00 %	95.44 %	
7.000	2.25	0.00 %	4.54 %	0.00 %	95.46 %	
7.400	2.25	0.00 %	4.54 %	0.00 %	95.46 %	Blood pH
8.000	2.25	0.00 %	4.54 %	0.00 %	95.46 %	
9.000	2.25	0.00 %	4.54 %	0.00 %	95.46 %	
10.000	2.25	0.00 %	4.54 %	0.00 %	95.46 %	
11.000	2.25	0.00 %	4.54 %	0.00 %	95.46 %	
12.000	2.25	0.00 %	4.54 %	0.00 %	95.46 %	

Carbonate and acidity

Carbonate 0.129 mM
Acidity error -0.811 mM

Other graphs

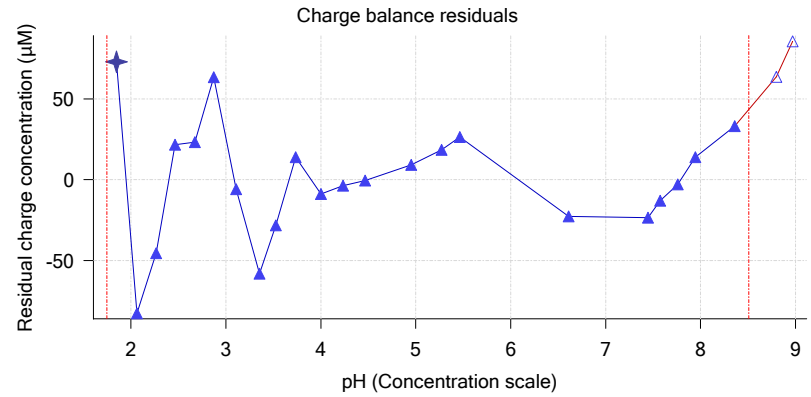


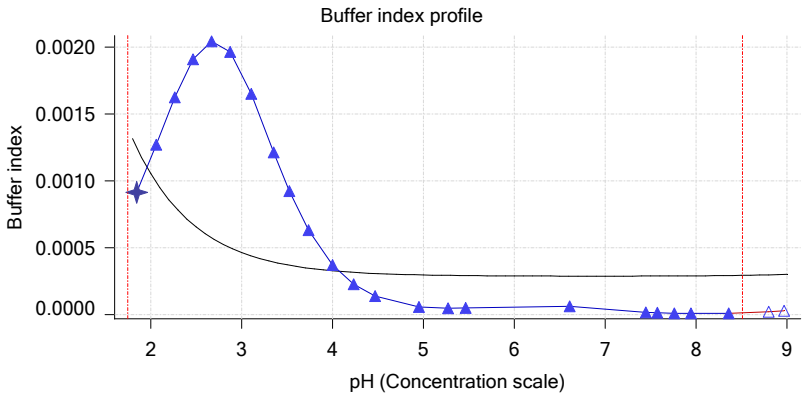


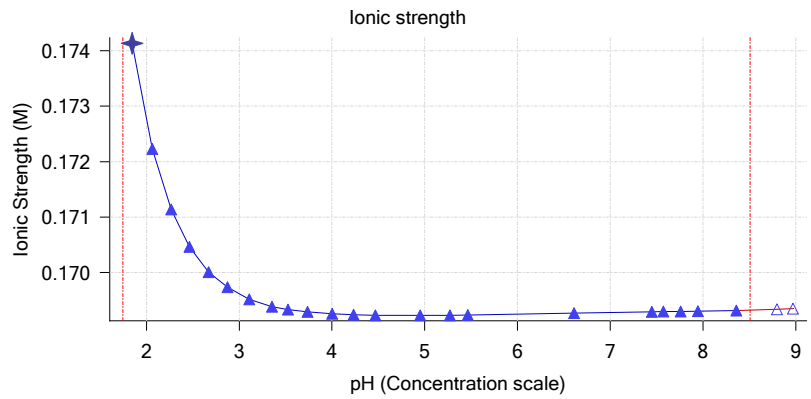
Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

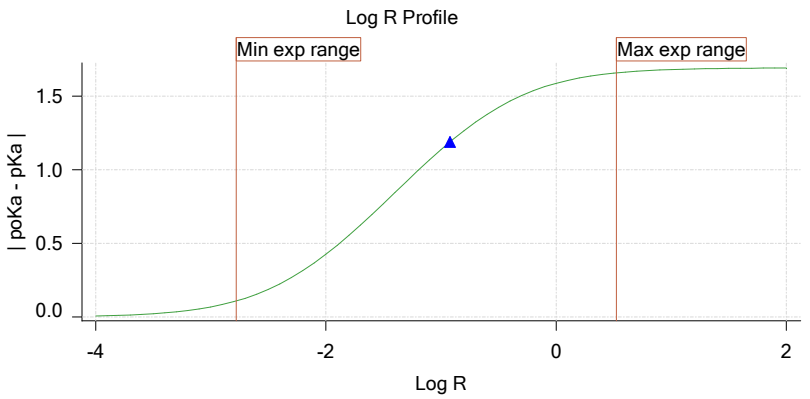
Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

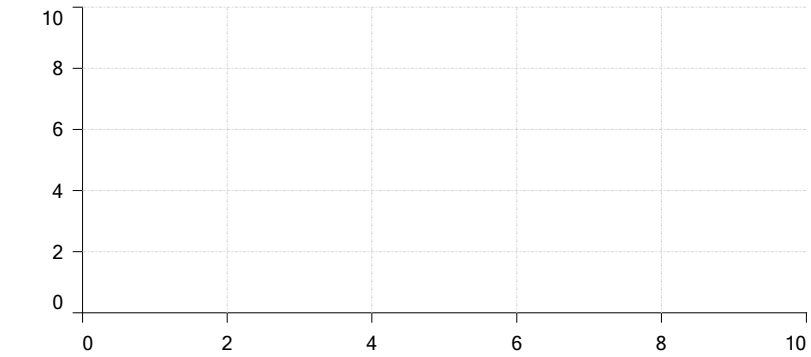
Other graphs (continued)

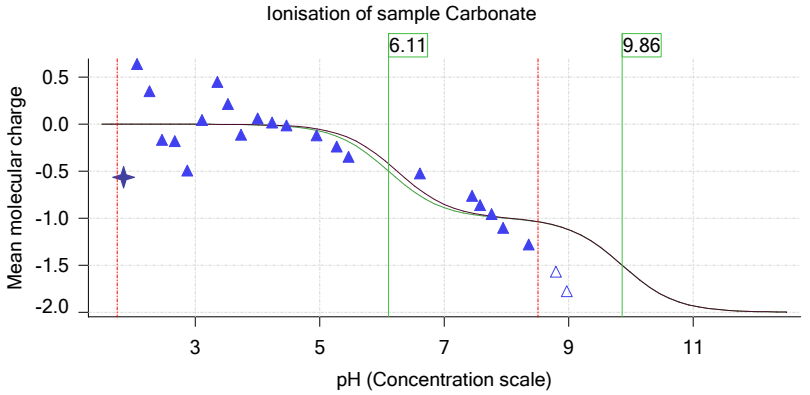












Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M11_octanol	2/27/2018 5:54:30 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001520 g	3/9/2018 2:22:09 PM	User entered value
Formula weight	211.22 g/mol	2/27/2018 5:54:30 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	211.22	2/27/2018 5:54:30 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 5:54:30 PM	User entered value
Sample is a	Base	2/27/2018 5:54:30 PM	User entered value
pKa 1	3.89	2/27/2018 5:54:30 PM	User entered value
logp (XH +)	0.55	3/2/2018 4:29:35 PM	User entered value
logP (neutral X)	2.19	3/2/2018 4:29:30 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
5:00.2	Initial pH = 9.10									
7:59.8	Data point 1	1.50000 mL	0.05315 mL	0.00268 mL	0.01999 mL	2.037	-0.00511	0.30733	0.00046	10.0 s
8:46.1	Data point 2	1.50000 mL	0.05315 mL	0.01642 mL	0.01999 mL	2.256	0.00288	0.69530	0.00017	10.5 s
9:22.2	Data point 3	1.50000 mL	0.05315 mL	0.02491 mL	0.01999 mL	2.463	0.00374	0.32148	0.00033	10.0 s
9:57.8	Data point 4	1.50000 mL	0.05315 mL	0.03048 mL	0.01999 mL	2.655	0.00078	0.10371	0.00012	10.5 s
10:33.9	Data point 5	1.50000 mL	0.05315 mL	0.03452 mL	0.01999 mL	2.854	-0.00337	0.19592	0.00038	10.0 s
11:09.3	Data point 6	1.50000 mL	0.05315 mL	0.03765 mL	0.01999 mL	3.078	0.00146	0.01563	0.00058	10.5 s
11:45.3	Data point 7	1.50000 mL	0.05315 mL	0.04026 mL	0.01999 mL	3.271	-0.00477	0.53594	0.00032	10.0 s
12:20.8	Data point 8	1.50000 mL	0.05315 mL	0.04264 mL	0.01999 mL	3.480	-0.00721	0.85954	0.00038	10.0 s
12:56.3	Data point 9	1.50000 mL	0.05315 mL	0.04478 mL	0.01999 mL	3.707	-0.01214	0.77245	0.00068	10.5 s
13:32.3	Data point 10	1.50000 mL	0.05315 mL	0.04657 mL	0.01999 mL	3.912	-0.01020	0.53326	0.00069	10.0 s
14:07.7	Data point 11	1.50000 mL	0.05315 mL	0.04798 mL	0.01999 mL	4.094	-0.00754	0.73914	0.00043	10.0 s
14:43.1	Data point 12	1.50000 mL	0.05315 mL	0.04908 mL	0.01999 mL	4.274	-0.01378	0.67663	0.00083	10.0 s
15:18.5	Data point 13	1.50000 mL	0.05315 mL	0.04988 mL	0.01999 mL	4.454	-0.01794	0.90958	0.00093	16.5 s
16:00.3	Data point 14	1.50000 mL	0.05315 mL	0.05047 mL	0.01999 mL	4.635	-0.01742	0.86808	0.00092	15.0 s
16:40.7	Data point 15	1.50000 mL	0.05315 mL	0.05087 mL	0.01999 mL	4.824	-0.01787	0.84622	0.00096	24.5 s
17:30.7	Data point 16	1.50000 mL	0.05315 mL	0.05115 mL	0.01999 mL	5.023	-0.01827	0.90373	0.00095	21.0 s
18:17.2	Data point 17	1.50000 mL	0.05315 mL	0.05134 mL	0.01999 mL	5.193	-0.01878	0.91929	0.00097	23.0 s
19:10.8	Data point 18	1.50000 mL	0.05315 mL	0.05155 mL	0.01999 mL	5.715	-0.01901	0.96541	0.00096	37.0 s
20:18.6	Data point 19	1.50000 mL	0.05315 mL	0.05174 mL	0.01999 mL	6.941	-0.08865	0.99621	0.00438	Timed out at 59.5 s
21:54.2	Data point 20	1.50000 mL	0.05315 mL	0.05181 mL	0.01999 mL	7.267	-0.07065	0.99539	0.00350	Timed out at 59.5 s
23:29.8	Data point 21	1.50000 mL	0.05315 mL	0.05188 mL	0.01999 mL	7.738	-0.08731	0.99760	0.00432	Timed out at 59.5 s
25:00.3	Data point 22	1.50000 mL	0.05315 mL	0.05193 mL	0.01999 mL	8.184	-0.04618	0.99543	0.00229	Timed out at 59.5 s
26:36.0	Data point 23	1.50000 mL	0.05315 mL	0.05200 mL	0.01999 mL	8.628	-0.02509	0.99264	0.00124	Timed out at 59.5 s
28:11.7	Data point 24	1.50000 mL	0.05315 mL	0.05212 mL	0.01999 mL	9.017	-0.01906	0.93147	0.00097	40.5 s
29:51.6	Data point 25	1.50000 mL	0.11291 mL	0.05212 mL	0.06999 mL	1.966	0.00082	0.01226	0.00037	10.5 s
30:38.4	Data point 26	1.50000 mL	0.11291 mL	0.06950 mL	0.06999 mL	2.173	-0.00810	0.69034	0.00048	10.5 s
31:14.6	Data point 27	1.50000 mL	0.11291 mL	0.08090 mL	0.06999 mL	2.379	0.00330	0.80719	0.00018	10.0 s
31:50.1	Data point 28	1.50000 mL	0.11291 mL	0.08841 mL	0.06999 mL	2.580	-0.01357	0.47607	0.00097	14.0 s
32:29.7	Data point 29	1.50000 mL	0.11291 mL	0.09374 mL	0.06999 mL	2.779	-0.00359	0.57678	0.00023	10.0 s
33:05.2	Data point 30	1.50000 mL	0.11291 mL	0.09781 mL	0.06999 mL	2.960	-0.00538	0.43414	0.00040	10.0 s
33:40.7	Data point 31	1.50000 mL	0.11291 mL	0.10115 mL	0.06999 mL	3.200	-0.01650	0.90031	0.00086	10.5 s
34:27.1	Data point 32	1.50000 mL	0.11291 mL	0.10362 mL	0.06999 mL	3.397	-0.00830	0.30538	0.00074	10.0 s
35:02.5	Data point 33	1.50000 mL	0.11291 mL	0.10569 mL	0.06999 mL	3.587	-0.01081	0.29933	0.00098	10.0 s
35:38.0	Data point 34	1.50000 mL	0.11291 mL	0.10729 mL	0.06999 mL	3.805	-0.00516	0.79057	0.00029	10.0 s
36:13.4	Data point 35	1.50000 mL	0.11291 mL	0.10842 mL	0.06999 mL	4.034	-0.00755	0.89227	0.00039	10.0 s

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
36:48.8	Data point 36	1.50000 mL	0.11291 mL	0.10915 mL	0.06999 mL	4.284	-0.01862	0.91237	0.00096	10.0 s
37:29.3	Data point 37	1.50000 mL	0.11291 mL	0.10960 mL	0.06999 mL	4.498	-0.01521	0.66710	0.00092	25.0 s
38:19.8	Data point 38	1.50000 mL	0.11291 mL	0.10988 mL	0.06999 mL	4.754	-0.01754	0.82634	0.00095	20.5 s
39:10.7	Data point 39	1.50000 mL	0.11291 mL	0.11018 mL	0.06999 mL	5.255	-0.01812	0.84415	0.00097	30.0 s
40:16.4	Data point 40	1.50000 mL	0.11291 mL	0.11035 mL	0.06999 mL	5.724	-0.01903	0.93383	0.00097	35.5 s
41:22.4	Data point 41	1.50000 mL	0.11291 mL	0.11042 mL	0.06999 mL	6.316	-0.03790	0.98438	0.00188	Timed out at 59.5 s
42:53.0	Data point 42	1.50000 mL	0.11291 mL	0.11056 mL	0.06999 mL	7.814	-0.06409	0.99645	0.00317	Timed out at 59.5 s
44:28.6	Data point 43	1.50000 mL	0.11291 mL	0.11070 mL	0.06999 mL	8.652	-0.02006	0.98249	0.00100	46.0 s
45:50.3	Data point 44	1.50000 mL	0.11291 mL	0.11082 mL	0.06999 mL	8.905	-0.01828	0.84297	0.00098	38.5 s
46:59.3	Data point 45	1.50000 mL	0.11291 mL	0.11091 mL	0.06999 mL	9.073	-0.01775	0.86902	0.00094	27.5 s
48:28.6	Data point 46	1.50000 mL	0.17582 mL	0.11091 mL	0.21999 mL	1.960	-0.00614	0.61144	0.00039	10.0 s
49:14.9	Data point 47	1.50000 mL	0.17582 mL	0.13074 mL	0.21999 mL	2.169	0.01032	0.30311	0.00093	10.0 s
49:50.6	Data point 48	1.50000 mL	0.17582 mL	0.14341 mL	0.21999 mL	2.367	-0.00532	0.40508	0.00041	10.0 s
50:26.1	Data point 49	1.50000 mL	0.17582 mL	0.15214 mL	0.21999 mL	2.563	-0.00517	0.08291	0.00089	10.5 s
51:02.2	Data point 50	1.50000 mL	0.17582 mL	0.15837 mL	0.21999 mL	2.768	-0.00887	0.21333	0.00095	10.0 s
51:37.8	Data point 51	1.50000 mL	0.17582 mL	0.16289 mL	0.21999 mL	2.967	0.00295	0.02140	0.00100	10.0 s
52:13.3	Data point 52	1.50000 mL	0.17582 mL	0.16625 mL	0.21999 mL	3.200	-0.00340	0.17172	0.00041	10.0 s
52:48.8	Data point 53	1.50000 mL	0.17582 mL	0.16860 mL	0.21999 mL	3.446	-0.01379	0.46424	0.00100	10.0 s
53:29.5	Data point 54	1.50000 mL	0.17582 mL	0.16992 mL	0.21999 mL	3.617	0.01450	0.85818	0.00077	33.5 s
54:43.8	Data point 55	1.50000 mL	0.17582 mL	0.17110 mL	0.21999 mL	3.827	-0.00092	0.01708	0.00035	10.5 s
55:19.9	Data point 56	1.50000 mL	0.17582 mL	0.17180 mL	0.21999 mL	4.090	0.00886	0.25159	0.00087	10.5 s
56:00.9	Data point 57	1.50000 mL	0.17582 mL	0.17222 mL	0.21999 mL	4.321	-0.01922	0.95151	0.00097	11.5 s
56:37.7	Data point 58	1.50000 mL	0.17582 mL	0.17248 mL	0.21999 mL	4.556	-0.01818	0.96232	0.00092	21.5 s
57:29.8	Data point 59	1.50000 mL	0.17582 mL	0.17277 mL	0.21999 mL	5.036	-0.00086	0.00356	0.00071	14.0 s
58:19.3	Data point 60	1.50000 mL	0.17582 mL	0.17288 mL	0.21999 mL	5.357	-0.01461	0.57206	0.00095	16.0 s
59:10.9	Data point 61	1.50000 mL	0.17582 mL	0.17295 mL	0.21999 mL	5.549	-0.01615	0.98210	0.00080	29.5 s
1:00:11.1	Data point 62	1.50000 mL	0.17582 mL	0.17307 mL	0.21999 mL	6.690	-0.09840	0.99748	0.00486	Timed out at 59.5 s
1:01:41.6	Data point 63	1.50000 mL	0.17582 mL	0.17319 mL	0.21999 mL	7.526	-0.12365	0.99119	0.00614	Timed out at 59.5 s
1:03:12.0	Data point 64	1.50000 mL	0.17582 mL	0.17324 mL	0.21999 mL	7.651	-0.08733	0.99550	0.00433	Timed out at 59.5 s
1:04:42.5	Data point 65	1.50000 mL	0.17582 mL	0.17328 mL	0.21999 mL	7.837	-0.13623	0.43667	0.01018	Timed out at 59.5 s
1:06:18.2	Data point 66	1.50000 mL	0.17582 mL	0.17335 mL	0.21999 mL	8.021	-0.06575	0.99623	0.00325	Timed out at 59.5 s
1:07:53.8	Data point 67	1.50000 mL	0.17582 mL	0.17345 mL	0.21999 mL	8.434	-0.11867	0.41261	0.00912	Timed out at 59.5 s
1:09:29.4	Data point 68	1.50000 mL	0.17582 mL	0.17361 mL	0.21999 mL	8.870	-0.01721	0.79761	0.00095	21.0 s
1:10:26.0	Data point 69	1.50000 mL	0.17582 mL	0.17373 mL	0.21999 mL	9.041	-0.01672	0.74463	0.00096	15.5 s
1:10:50.6	Assay volumes	1.50000 mL	0.17582 mL	0.17373 mL	0.21999 mL					

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	60 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.050 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09010_M11_octanol_pH-metric high logP.t3r**
Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.150 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.102	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus S	0.9967	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus jH	1.2	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus jOH	0.0	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r
Base concentration factor	1.000	3/9/2018 4:01:24 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	1.000	3/9/2018 4:01:24 PM	C:\Sirius_T3\HCl18C09.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 11:05:59 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 11:27:22 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 11:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	02-08-2018	3/6/2018 10:28:59 AM
Port B	Cyclohexane	11-01-17	2/27/2018 11:37:57 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 11:18:04 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09010**
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Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 10:59:35 AM
Titrator		T3TM1200161	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 3:01:00 PM
E0 calibration	+6.40 mV		3/9/2018 4:01:52 PM
Filling solution	3M KCl	KCL097	3/9/2018 11:05:42 AM
Liquids			
Wash 1	50% IPA:50% Water		3/9/2018 11:04:22 AM
Wash 2	0.5% Trition X-100 in H20		3/9/2018 11:04:25 AM
Buffer position 1	pH7 Wash		3/9/2018 11:04:27 AM
Buffer position 2	pH 7		3/9/2018 11:04:30 AM
Storage position			3/9/2018 11:05:04 AM
Wash water	5.3e+003 mL	02-27-2018	2/27/2018 10:54:39 AM
Waste	1e+004 mL		11/28/2017 11:36:29 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		074811	11/23/2010 12:22:28 PM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	123:16:41		11/23/2010 12:22:28 PM
Calibrated on	2/27/2018 11:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M11_octanol**
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Experiment start time: **3/9/2018 4:01:24 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00